Microscopic modeling of interface roughness scattering and application to the simulation of quantum cascade lasers

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Introduction / Abstract

The theory of interface roughness (IFR) scattering in semiconductor heterostructures is well established in the case of idealized abrupt interfaces [1]. However, in reality, interfaces have a finite width, i.e. interfaces are graded. In such case, the effect of interface roughness, i.e. the breaking of in-plane invariance, a general framework has been lacking to describe the induced scattering processes.

We have developed a more general model of IFR scattering applicable in presence of grading of the interfaces [2]. We have applied it to the simulation of quantum cascade lasers (QCLs). An important consequence is that the grading tends to reduce the effect of interface roughness and can be exploited as a resource to improve the QCL performances.

1. General theory of interface roughness

The interface roughness, which breaks the in-plane invariance of layer heterostructures, is usually parametrized by two parameters in the assumption of abrupt interfaces, namely the root-mean-square deviation Δ, and in-plane correlation length $\Lambda_{\parallel}$. In presence of grading, a third parameter is needed, the correlation length along the growth direction $\Lambda_{\perp}$. Experimental atom-probe tomography measurements on Ge/SiGe interfaces show that this axial correlation length can be smaller than the interfacial width. We have derived a general expression of the IFR scattering rate as a function of the correlation lengths and interface width.

2. Effect of interface roughness in the simulations of QCLs

We have implemented our general model for IFR scattering in a non-equilibrium Green's function simulator (nextnano.NEGF) through the inclusion of the corresponding self-energy. For a proposed Ge/Si-Ge-based quantum cascade laser, the impact of IFR scattering is strongly reduced and the estimated maximum gain is found to be twice larger than in the abrupt case model. We show that our model gives further insights into the simulation of various devices, ranging from THz to mid-infrared and short-wavelength QCLs, and the prediction of their performances in terms of current threshold, maximum operating temperature, and output power.

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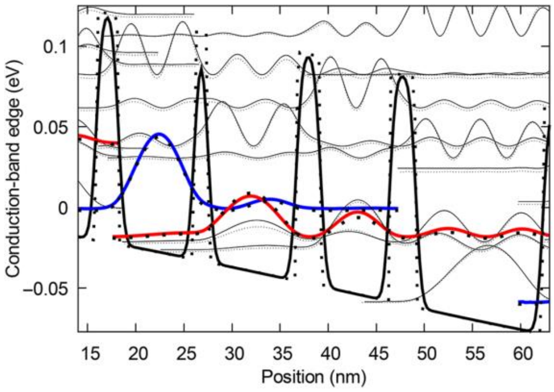

Fig. 1: Bandedge and electronic states of a THz *n*-type Ge/SiGe QCL with abrupt interfaces (dashed lines) and with gradded interfaces (solid lines). Squared wave functions associated with the upper (ULL, blue) and lower laser levels (LLL, red) are highlighted.

References

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